

Probing Nanomagnetism with Neutrons and Advanced Simulations

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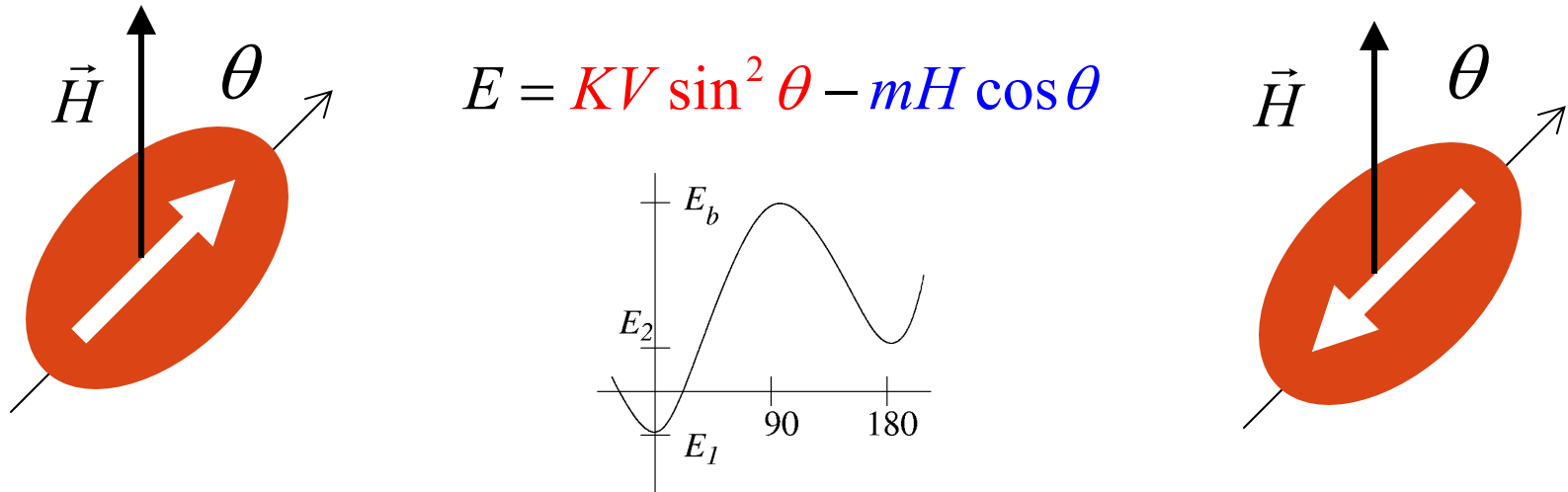
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Why nanomagnetism in this talk?

- **Because it is important!**
 - True applications of nanoscience already exist!
- **Because it can serve as a model for other fields**

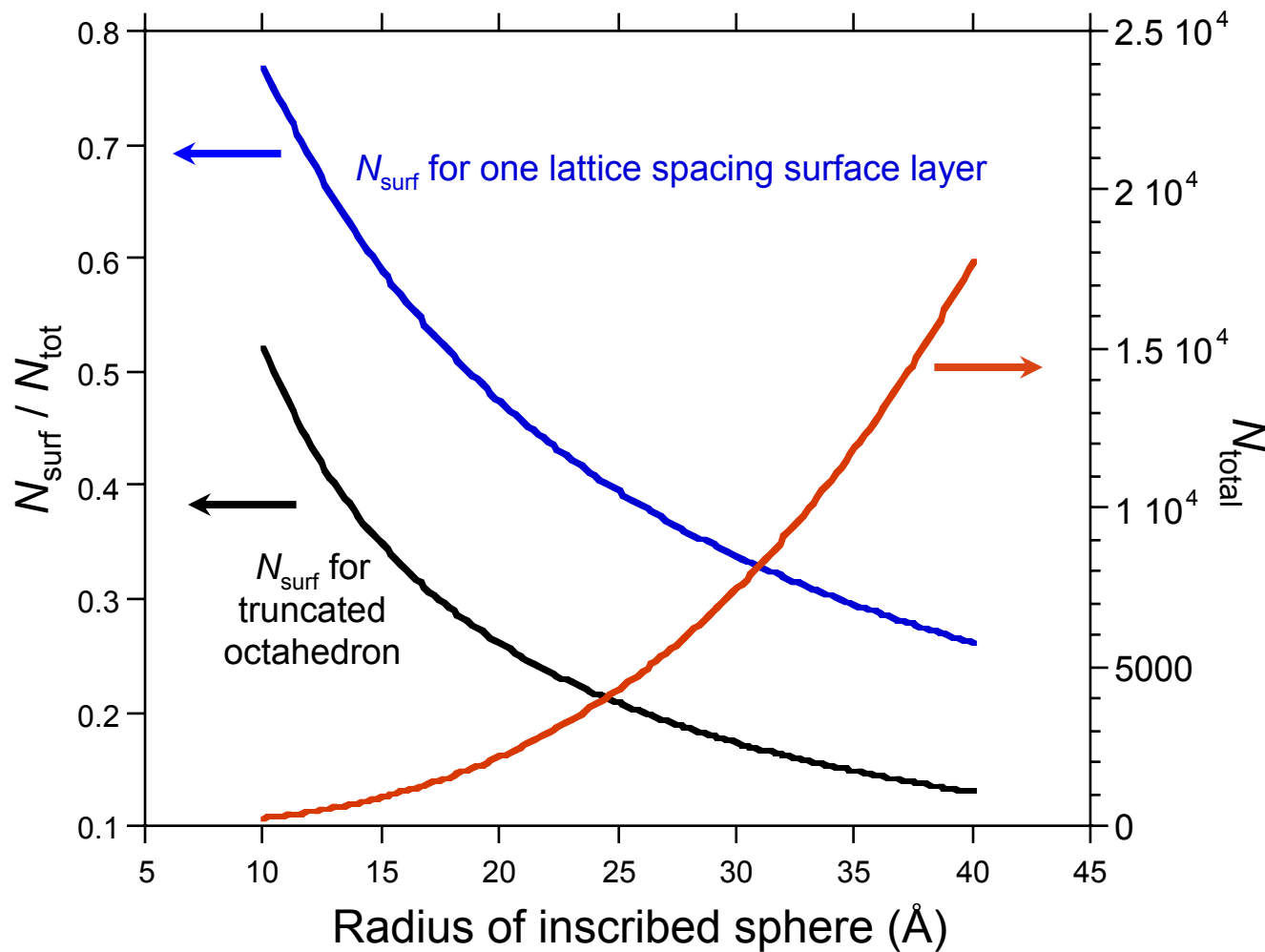
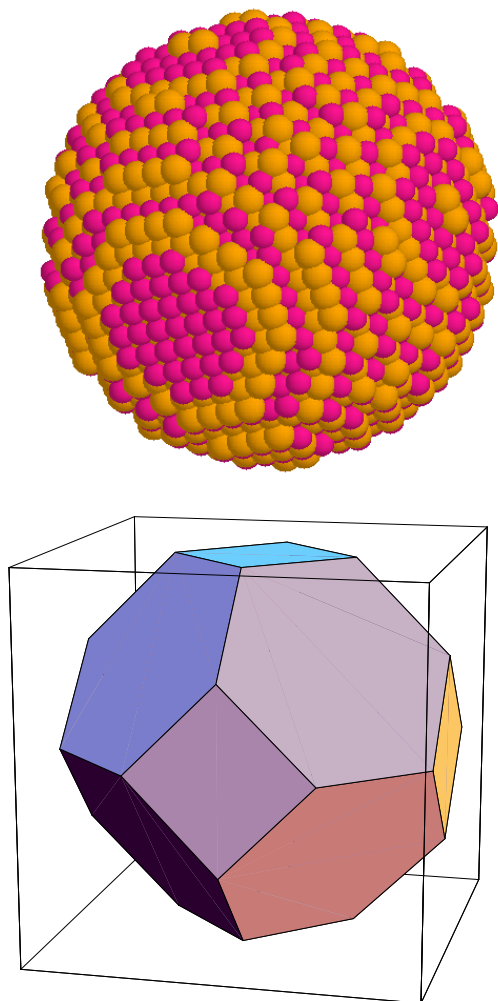
Example: Information storage in nano-grains and particles

(see Eric Fullerton's talk, yesterday)



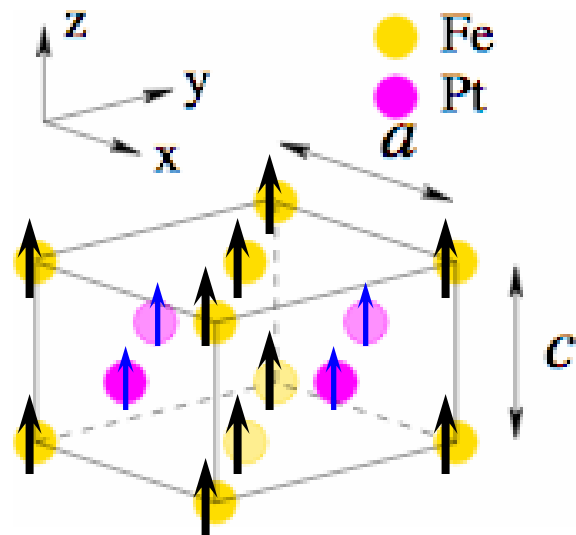
- Thermal stability requires energy barrier constant energy barrier
 - Reduce volume means increase anisotropy
- FePt nanoparticles with 5nm diameter (10-100 Tb/in²)
 - Can be synthesized and are “hard” enough
- But presently it is not known how to write data
 - **Needed is a detailed understanding of reversal process**

Example: FePt (L10) Nanoparticle



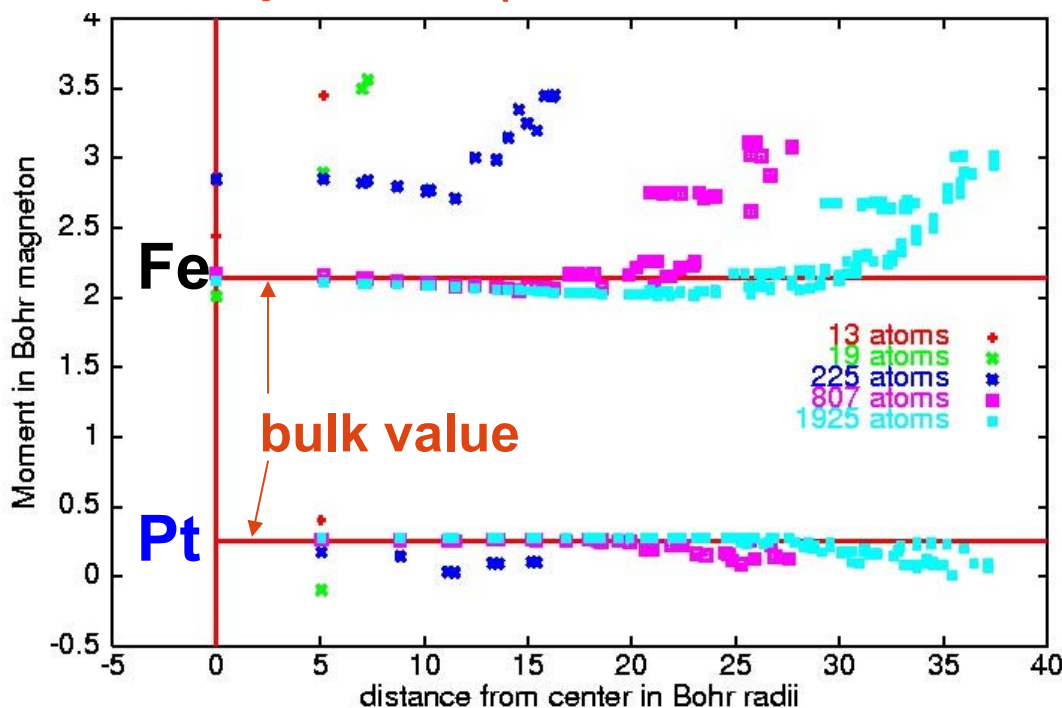
⇒ **Nanoscale is dominated by interface**

Calculating the magnetic structure in nanoparticles from first principles



Small induced moment on Pt responsible for the magnetic coupling

Calculated moments for 13, 19, 225, 807, and 1925 atom particles (Nicholson & Eisenbach)



Magnetic structure in nanoparticle is much more complex than in the bulk

Surface Spin Disorder in Nanoparticles

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Surface Spin Disorder in NiFe_2O_4 Nanoparticles

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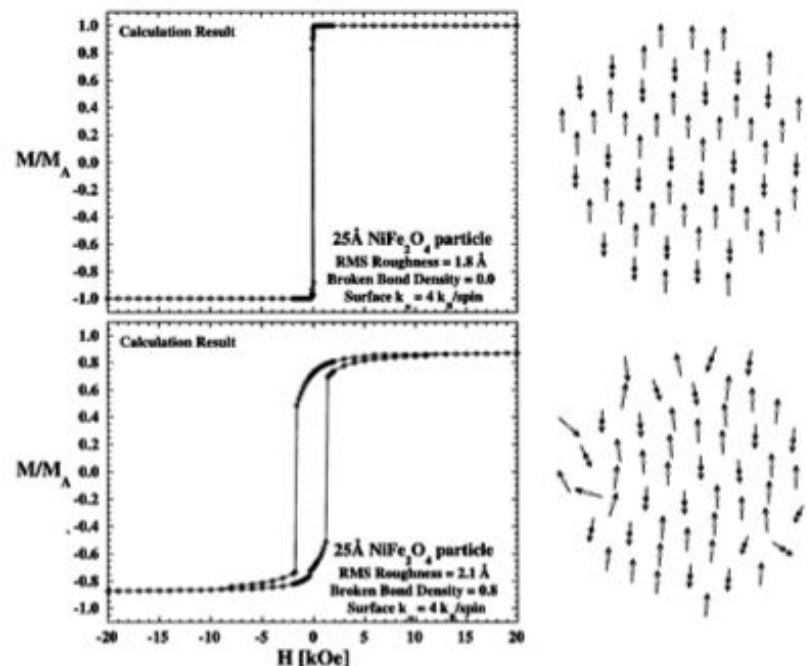
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Nickel ferrite nanoparticles exhibit anomalous magnetic properties at low temperatures: low magnetization with a large differential susceptibility at high fields, hysteresis loops which are open up to 160 kOe, time-dependent magnetization in 70 kOe applied field, and shifted hysteresis loops after field cooling. We propose a model of the magnetization within these particles consisting of ferrimagnetically aligned core spins and a spin-glass-like surface layer. We find that qualitative features of this model are reproduced by a numerical calculation of the spin distribution. Implications of this model for possible macroscopic quantum tunneling in these materials are discussed. [S0031-9007(96)00628-X]

PACS numbers: 75.50.Tt, 75.30.Pd, 75.50.Gg, 75.50.Lk

- Competition between surface anisotropy and exchange
- Maybe even random exchange
- Ferro- (Ferri-) magnetic interior couples to spin-glass (antiferromagnetic) surface region
- Enhancement of “effective” anisotropy

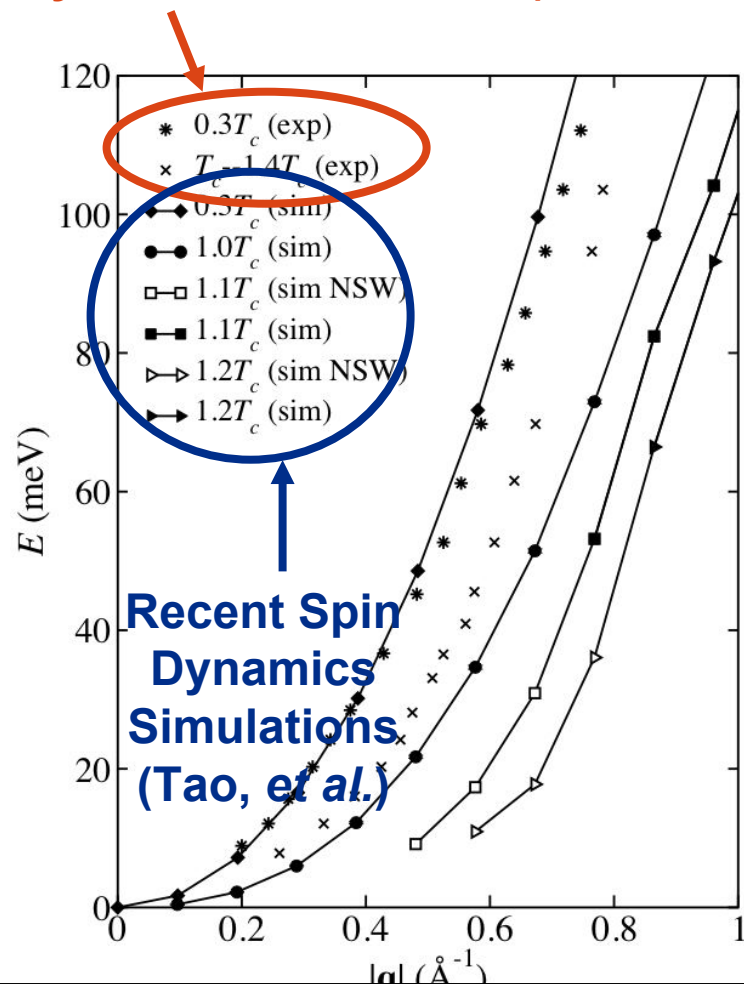


Complexity at the atomic and nano-scale changes the magnetic properties!

Where do neutrons come in?

- Besides structure neutrons probe dynamic response: $S(q, \omega)$
- Explore magnetic excitations
 - Intra particle/grain
 - Inter particle/grain
- Simulations help make sense of $S(q, \omega)$
 - generate pictures / movies
- Tune spin-models for nanostructures by comparing simulations and inelastic experiment

Spins Waves in Paramagnetic Iron (Exp. Lynn and Mook, 1970s)



Simulating up to 10^6 moments possible
(hundreds of interacting nanoparticles)

Summary: the role of neutron scattering and advanced simulations

Neutron scattering experiments:
 $S(q)$ and $S(q, \omega)$

**Knowledge, new effects,
models that predict properties and
assist design of new
nanostructures**

Ab initio calculations:

- structure
- short dynamics

Spin models:

- dynamics
- ensembles

For the discussion

Should theory, modeling, and simulations remain a single PI endeavor?

**What is badly needed is
“computational instrumentation”**